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14. ABSTRACT

This research project pursues basic understanding of rarefied gas flows, leading to Air Force tools for plumes, spacecraft, and micro-devices. It develops, applies, and validates kinetic and molecular-level models of improved physical realism for nonequilibrium processes such as collisional interaction of gases, gas-particulate mixtures, and gas surface interaction that arise in high temperature, multi-species, chemically reacting rarefied flowfields such as rocket plumes. These phenomena are not accurately addressed by standard engineering tools and require improved understanding of the basic physics. A number of closely related research issues arise in the area of rarefied flows on the micro length scales, including micropropulsion flows. The key computational tool used in this effort is the direct simulation Monte Carlo (DSMC) method and related kinetic solvers. Recently, a 3D multi-phase DSMC capability has been developed and applied to study the interaction of solid propellant plumes with rarefied atmosphere. A parallel 3D Monte Carlo numerical tool for modeling radiation in multi-phase flows has been developed; the integration of fluid and radiation tools is planned in the future. New optical micropropulsion concepts have been formulated based on non-resonant interaction of optical lattice and carrier gas. Spacecraft contamination effects have been studied, and efficient numerical models for surface roughness were proposed.

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1. Title: Plume Simulation, Contamination, and Microfluidics (Preprint)

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2. Abstract: *This research project pursues basic understanding of rarefied gas flows, leading to Air Force tools for plumes, spacecraft, and micro-devices. It develops, applies, and validates kinetic and molecular-level models of improved physical realism for nonequilibrium processes such as collisional interaction of gases, gas-particulate mixtures, and gas surface interaction that arise in high temperature, multi-species, chemically reacting rarefied flowfields such as rocket plumes. These phenomena are not accurately addressed by standard engineering tools and require improved understanding of the basic physics. A number of closely related research issues arise in the area of rarefied flows on the micro length scales, including micropropulsion flows. The key computational tool used in this effort is the direct simulation Monte Carlo (DSMC) method and related kinetic solvers. Recently, a 3D multi-phase DSMC capability has been developed and applied to study the interaction of solid propellant plumes with rarefied atmosphere. A parallel 3D Monte Carlo numerical tool for modeling radiation in multi-phase flows has been developed; the integration of fluid and radiation tools is planned in the future. New optical micropropulsion concepts have been formulated based on non-resonant interaction of optical lattice and carrier gas. Spacecraft contamination effects have been studied, and efficient numerical models for surface roughness were proposed.*

3.1 Research Highlights

A. Multi-Phase Flows:

Find, Fix, Track, Target, Engage and Assess (F2T2EA) – AF/MDA systems use IR sensors – particulates, soot, droplets can dominate the signature

During FY06, this task performed sensitivity studies on a two-phase plume flow expanding from a 140 N aluminized solid propellant thruster into vacuum, using continuum and kinetic approaches. Comparison of the four predictions (three continuum and one kinetic) have shown very good agreement for gas-only flows, both with constant and variable number of internal degrees of freedom. When alumina particles were included in the simulation, there was disagreement between the three continuum solutions. The two-phase solutions obtained by SMILE and CFD++ agree very well, as shown in Fig. 1, except for particle temperature distributions in the plume. The latter one differs due to the differences in the gas-particle heat transfer rates. The applicability of gas-to-particle heat transfer correlations used in CFD++ to the free-molecular and near-free-molecular flow regime typical for micron-sized particles in the plume is questionable and needs to be further investigated. On the other hand, the expressions used in the DSMC model are accurate for the free-molecular regime, but have adjustable parameters, namely, translational and internal energy accommodation coefficients. The studies showed significant dependence of particle temperature on energy accommodation coefficient, which illustrates the importance of reliable data on translational and internal energy accommodation coefficients for gas molecules colliding with hot particle surfaces, see figure 2.

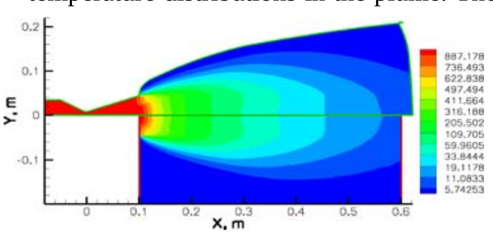


Figure 1. Comparison of continuum (CFD++, top) and kinetic (SMILE, bottom) pressure fields (Pa) for a gas-only flow

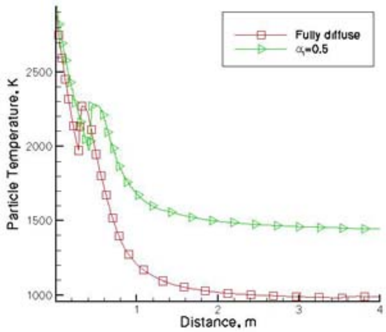


Figure 2. Particulates in plume cool faster if gas accommodation value is higher

A nonequilibrium alumina phase change model has been implemented in the two-phase DSMC code, and was shown to qualitatively predict experimental results on particle temperature evolution during the phase change. The phase change impact on particle temperature was very significant, and accurate modeling of this process is needed both for the continuum and kinetic approaches. The phase change is expected to occur in the nozzle for sub-micron particles, and in the plume for larger particles. It is important that particles mostly freeze in the meta-stable γ phase when gas cooling is the main mechanism of temperature decrease, and in the stable crystalline α phase when they are radiatively cooled.

During FY07, simulations of two-phase rocket motors interacting with atmosphere at hypersonic velocities and altitudes over 100 km will be performed along with radiation overlay predictions that can be compared with measured UV and IR data. This should provide improved understanding of the importance of radiation scattering and gas-particle accommodation assumptions. Simulations of two-phase rarefied flows containing liquid droplets will be initiated, looking at sensor blinding and contamination issues by utilizing simple condensation models from the literature along with our new two-phase transport capability.

B. Plume Radiation Model

During FY06, a parallel 3D line-by-line (molecular rotational line) radiation transport code has been developed based on the Monte Carlo photon-tracing approach and aimed at accurate prediction of radiation from rocket plumes, accounting for flow nonequilibrium and both gas and particulate phases. To the best of our knowledge, this is the first 3D line-by-line nonequilibrium radiation code available. The code is currently

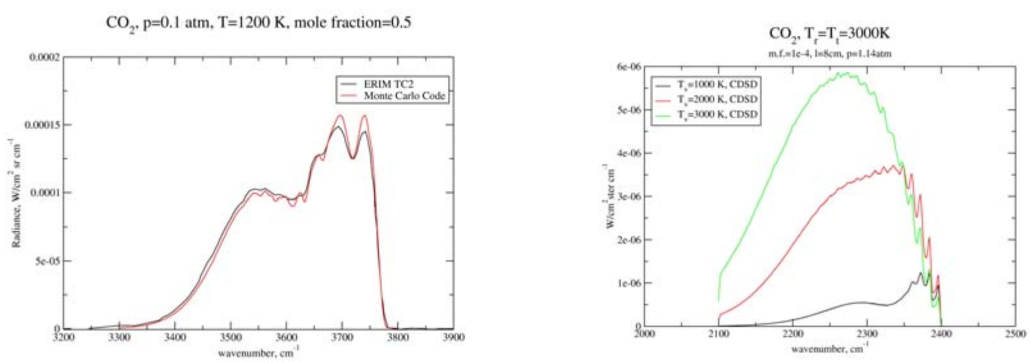


Figure 3. Equilibrium and two-temperature radiation simulations

being tested and its validation through comparisons with available experimental data is under way. **Among other things, this code will enable the plume radiation predictions described above.**

The calculation of gas absorption coefficient is made more efficient by using a special procedure where the number of times the line function must be evaluated is reduced by interpolating over regions where the contribution from a particular line function varies smoothly. To this end, the code employs a binary grid division and conducts piecewise calculations across a series of cascaded grids. The particle absorption and scattering coefficients are calculated using Mie theory and the correlations for real and imaginary parts of the complex refraction index given by Plastinin et al and Dombrovsky. The particle scattering phase function is calculated using Henyey-Greenstein approximation. The radiation code takes into account the nonequilibrium between translational, rotational, and vibrational modes, where the line intensity is calculated according to equilibrium rotational and vibrational populations at given rotational and vibrational temperatures. The Voigt line shape function is used with the parameters calculated using the gas translational temperature. Comparison of the computed and measured radiation in equilibrium heated gas cell is given in the figure above. The result shows good agreement between numerical modeling and experimental data. The impact of gas nonequilibrium on IR radiation is very significant, as shown in the figure above. The importance of energy accommodation coefficients mentioned in Section A is clearly shown in Fig 3 where the radiance from a two-phase plume of a 140 N aluminized propellant thruster is calculated in the direction perpendicular to the plume axis at a location close to the exit plane. The complete accommodation of energy of gas molecules on the particulate surface results in lower surface temperature (about 2200K), while an incomplete accommodation (corresponds to the energy accommodation coefficient of 0.8) leads to warmer particles (about 2300K). The difference in particle temperature has a strong impact on the resulting radiance; note also that in this case the particle radiance is visibly stronger than that from the gas, making clear the vital necessity of the new two-phase plume simulation capability developed by this project

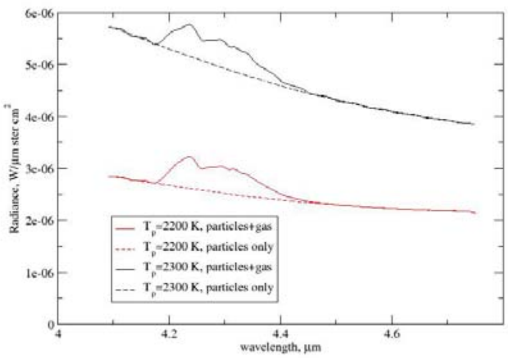


Figure 4. Radiation computed for two-phase plume case.

Extensive code validation and application to several plume/atmosphere interaction scenarios are being planned. The development of two-dimensional and axisymmetric modules of the radiation code that will allow us to achieve significantly better flow resolution is also in the plans. Work toward incorporation of accurate modern databases for carbon dioxide and water molecules is currently under consideration. An important topic for future consideration is also the interaction between parts A and B; the integration between our DSMC fluid solver and Monte Carlo radiation solver is being planned.

***C. Optical lattice interactions with gases**:*

Adapt and use rarefied gas flow (DSMC) simulation tools to estimate potential payoff of innovative laser-accelerated gas microthruster

During FY06, the DSMC method was used to study the feasibility of new propulsion concepts based on the interaction of an optical lattice with gas molecules. Two regimes were considered, high density and low density. In the first one, a de Laval nozzle was examined with the carrier gas driven by energy and momentum deposition from the lattice to the region near the nozzle throat. Analytical expressions were developed and compared with the numerical predictions, describing the energy and momentum energy transfer between the lattice and the gas for a cold microthruster influenced by intersecting laser beams with a pulse duration on the order of 50 ps. The thrust of the nozzle increases from 1.19mN for a flow without a lattice to 2.99mN for the flow with a lattice. The lattice effect on the specific impulse is smaller since the mass flow is also increased in the present configuration but the increase in specific impulse to 92s from 72s is still significant. The greatly enhanced performance of a cold gas thruster integrated with an optical lattice has been demonstrated and we point out

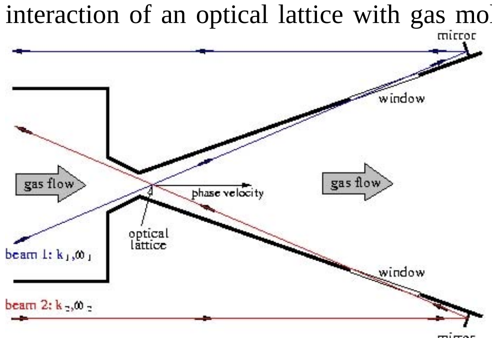


Figure 5. Schematic of high-density microthruster.

that a larger gas density, laser energy, and more laser pulses will result in subsequent increase in device performance both in terms of thrust and specific impulse.

In the second, nearly collisionless, regime, a multiple orifice flow was considered with molecules accelerated to high velocities by a chirped lattice potential. DSMC computations have been conducted to analyze the performance of the micropropulsion device. The optical lattice was created with two 800nm wavelength beams, the maximum laser intensity at the axis was $6.4 \times 10^{16} W/m^2$, and the pulse duration was 10ns. The carrier gas was methane, initially stagnant at pressure of 0.01torr and temperature of 300K. Large flow velocities at the exit plane result in significant improvement of the propulsion performance. The thrust increases from 3.4nN to 64nN, and the specific impulse increases 66s to 385s. Note that there is a potential for a several orders of magnitude increase in thrust and specific impulse (several times) when larger densities, higher laser intensities, multiple lattices and pulse re-utilization are used.

During FY07, this micro-thruster concept will be transitioned to PRSS if of interest, and other possible applications (such as species separation or materials processing) may be given cursory feasibility simulations. The impact of optical lattice on gas mixtures will be analyzed, with the potential application to study molecular cross sections for collision velocities from several to tens of kilometers per second. Another area of interest is energy deposition from optical lattice to high-density gas, when the gas temperature increases per thousands of degrees over a single laser pulse.

D. Plume Surface Interaction and Rough Surface Model.

Microfluid/micronozzle simulations must include effects of surface roughness -- first practical DSMC roughness model and experimental validation data are presented

During FY06, rarefied gas flows expanding into vacuum through 150 μm X 1.5 cm channels were studied experimentally, and numerically with the DSMC method. Different types of channel walls were examined, both polished and rough with well-characterized roughness shaped as triangles and rectangles. A new conical surface roughness model applicable for the DSMC method was proposed and verified. An expression relating this model to the Cercignani-Lampis scattering model has been derived. A significant impact of the surface roughness on mass flow through a channel was observed both experimentally and numerically. The mass flow in a rough channel is lower than that of a polished surface channel, with the difference amounting to 6% for larger pressures and 30% for smaller pressures. A good agreement between the numerical and experimental results is obtained for a rough surface channel, thus validating the conical roughness model.

During FY07, further validation cases for this model will be examined and micropropulsion-related flows will be simulated. Accurate experimental modeling of several rough surfaces is planned. A sophisticated surface roughness by Anolik is being analyzed and considered for examination in DSMC.

E. Kinetic modeling of thermal transpiration flows.

Rarefied flow devices (Knudsen compressor) may have payoff for Near-space -- research shows new numerical implementation of ES method has validated predictive capability, vastly higher speed

The phenomenon of temperature-driven gas flow in a channel (thermal transpiration) is the fundamental basis of the Knudsen compressor. A practical Knudsen compressor would have potentially significant AF applications, including direct-solar-powered near-space propulsion concepts. However, important improvements are needed in fundamental understanding before a practical version can be envisioned. During FY06, our simulation capabilities were greatly enhanced by the development of discrete ordinate methods for the solution of the ellipsoidal statistical (ES) and Bhatnagar-Gross-Krook (BGK) models. As demonstrations, DSMC, ES, and BGK simulations were used to numerically study rarefied gas flow through a two-dimensional, finite length channel. The discrete ordinate method for the ellipsoidal statistical model kinetic equation provides accurate numerical solutions of transpiration flow in a channel at a significantly lower computational cost compared to the DSMC method. As a further test case, a heated microbeam was simulated and the results showed good qualitative comparison with experimental data from Sandia Labs, at greatly reduced computational cost compared with DSMC.

The FY06 work is a first look at describing practical thermal gradient driven flows in Knudsen Compressors. The finite difference formulation used is being reconsidered, and its replacement by a much more general finite volume one is being planned both for two-dimensional and axisymmetric problems.

3.2 Relevance / Transitions

The results of this basic research program are clearly relevant to several aspects of the Air Force mission. Firstly, this project's research has generated and investigated new and improved methods for simulation of rarefied, reacting, two-phase gas flows, such as rocket, missile, or thruster plumes at high altitudes. These plumes typically include a large mass fraction of alumina particles (in the case of a solid rocket) or a substantial number fraction of soot particles (in the case of a liquid system). USAF programs such as SBIRS-high, as well as MDA programs (STSS, BPI, THAAD) rely on an accurate picture of the target or threat missile signature for all stages of flight. New Space Command needs for space situational awareness will also require tools for simulating satellite thrust plume-induced optical signatures and physical self- and cross-contamination. AFOSR-sponsored AFRL and University research has been transitioned to users for these programs for interceptor and algorithm development. Results from previous years have allowed DoD users to study the potential sensor self-blinding from a missile divert thruster side-jet plume, but the question has remained as to the validity of these results for a two-phase plume containing alumina, soot particles, or liquid drops. **The latest research results discussed here, including the first-ever 3D two-phase DSMC plume computation and integrated radiation module, now allow these important cases to be reasonably simulated.**

In addition to the plume signature uses, **these research results are being transitioned for satellite contamination studies.** As a demonstration, the first-ever full three-dimensional modeling of a nano-satellite plus thruster plume has been performed to predict contamination effects and force moments for the FMMR thrust on the AggieSat. Two locations of the FMMR were examined, the center of a cylinder panel and the edge of the panel. The de-spinning moment was found to be over 60% larger, and the contamination from the water vapor significantly less, for the second location. Future USAF missions, with increased use of nanosatellites and constellations, will require numerous contamination predictions and mitigation studies. Issues of contamination are expected to be particularly severe when the plume contains liquid droplets and requires a two-phase simulation tool.

The ultra-sensitive capabilities of the AFOSR-funded nano-Newton thrust stand has been used to perform measurements and **proof-of-concept studies for two DARPA nanopropulsion concepts**. One was an experimental MEMS digital nano-thruster concept funded by DARPA and Navy. The other was SRI's DARPA-funded micro-electric thruster concept.

The newly-developed capability to rapidly simulate low-velocity microfluids using the ES kinetic model has been transitioned to the Sandia National Laboratory and used to predict displacement of a heated microbeam in a practical MEMS device.

4. PUBLICATIONS

1. A paper from last year: "Performance testing of a microfabricated propulsion system for nanosatellite applications," **was recognized by** *Journal of Micromechanics and Microengineering*, for having been downloaded more than 500 times – more than 97% of all other papers.
2. Ahmed Z, Gimelshein SF, Ketsdever AD, Numerical analysis of free-molecule microresistojet performance, Journal of propulsion and power 22 (4): 749-756 JUL-AUG 2006
3. *O. Sazhin, A. Kulev, S. Borisov, and S. Gimelshein, Numerical analysis of gas-surface scattering effect on thermal transpiration, Submitted to Vacuum.*
4. **Invited article** *A.A. Alexeenko, S.F. Gimelshein, E.P. Muntz, A.D. Ketsdever, Kinetic Modeling of Temperature-Driven Flows in Short Microchannels, Int. J. of Thermal Sciences, In Press, Corrected Proof, Available online 9 March 2006.*
5. *T. C. Lilly, S.F. Gimelshein, A.D. Ketsdever, and G.N. Markelov, Measurements and computations of mass flow and momentum flux through short tubes in rarefied gases, To appear in Physics of Fluids.*

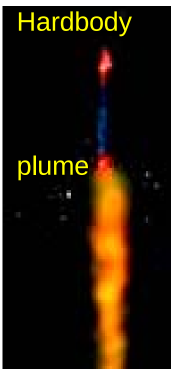
6. *M.N. Shneider, C. Ngalande, S.F. Gimelshein, Microscale thrusters with pulsed optical lattices / gas nonresonant dipole interaction, Submitted to Journal of Propulsion and Power.*
7. *M.N. Shneider, P.F. Barker, S.F. Gimelshein, Transport in room temperature gases induced by optical lattice, To appear in Journal of Applied Physics.*
8. *M.N. Shneider, S.F. Gimelshein, P.F. Barker, Micropropulsion devices based on molecular acceleration by pulsed optical lattices,Journal of Applied Physics, (AIP)99, no. 6, (15 March 2006) : 63102-1-5*
9. **Invited talk** *Y.-L. Han, A.A. Alexeenko, M. Young, E.P. Muntz, Experimental and Computational Studies of Temperature Gradient Driven Molecular Transport in Gas Flows through Nano/Micro-Scale Channels, 2nd International Conference on Transport Phenomena in Micro and Nanodevices, Barga, Italy, June 11-15, 2006. Submitted to Microscale Nanoscale Thermophysical Engineering, August 2006.*
10. *C. Ngalande, S.F. Gimelshein, and M.N. Shneider, Statistical Modeling of Interactions between Gas Molecules and Pulsed Optical Lattices, 25th International Symposium on Rarefied Gas Dynamics, 22-27 July 2006, St. Petersburg, Russia.*
11. *M.N. Shneider, C. Ngalande, S.F. Gimelshein, Micropropulsion devices with pulsed optical lattices / gas nonresonant dipole interaction, AIAA Paper 2006-768.*
12. *A.A. Alexeenko, E.P. Muntz, M. Gallis, and J.R. Torczynski, Comparison of Kinetic Models for Gas Damping of Moving Microbeams, AIAA Paper 2006-3715.*
13. *A.A. Alexeenko, Evaluation of Kinetic Models for Low-Speed Microscale Flows, International Symposium on Rarefied Gas Dynamics, Saint-Petersburg, Russia, July 20-28, 2006*
14. S. Gimelshein, G. Markelov, and J. Muylaert, Numerical Modeling of Low Thrust Solid Propellant Nozzles at High Altitudes , AIAA-2006-3273, 37th AIAA Plasmadynamics and Lasers Conference, San Francisco, California, June 5-8, 2006
15. T. Ozawa, D. Levin, and I. Wysong, O+HCl Chemistry Models for Hypervelocity Collisions in DSMC, AIAA-2006-1193, 44th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 9-12, 2006.
16. C. Ngalande, M. Shneider, S. Gimelshein, Collisional Molecular Transport in Pulsed Optical Lattices**,** AIAA-2006-2900, 37th AIAA Plasmadynamics and Lasers Conference, San Francisco, California, June 5-8, 2006
17. T. Ozawa, D. Levin, I.J. Wysong, O+HCl Cross sections and reaction probabilities in DSMC, 25th International Symposium on Rarefied Gas Dynamics, 22-27 July 2006, St. Petersburg, Russia.
18. N.E. Gimelshein, T.C. Lilly, S.F. Gimelshein, A.D. Ketsdever, I.J. Wysong,, Surface roughness effects in low reynolds number nozzle flows, 25th International Symposium on Rarefied Gas Dynamics, 22-27 July 2006, St. Petersburg, Russia.
19. M. Capitelli, I. Wysong, G. Capitta, and G. Colonna, A Model For Ammonia Solar Thermal Thruster, Journal of Thermophysics and Heat Transfer, in press.

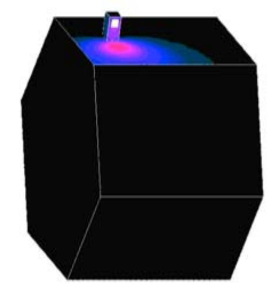
Plume Simulations, Contamination, Microflows at AFRL/PRSA

Goal: Pursue basic understanding of rarefied gas flows, leading to Air Force tools for plumes, spacecraft, and microdevices

Science topic

- Direct simulation Monte Carlo: 2-Phase Flows, molecular models, radiation
- Unsteady rarefied flows
- Gas-Surface interaction, Surface roughness models
- Plume-plume interactions, Low Re flows





AF application

- Plume IR signatures: tracking, identification, intercept algorithms, sensor design
- Contamination, sensor interference
- Micropropulsion flows

Transition

- MDA: SOCRATES-P
- FMMR (TAMUSat), microprop devices
- Advanced concepts: Near-space

Approach

DSMC, other kinetic methods, CHAFF vacuum facility, nano-Newton thrust stand

Plume Simulations, Contamination, Microflows: Partners

DOE/Sandia Lab: microdevices

Smith, MDA: plume code users

NASA: plume contamination, droplets

Dressler AFRL/VS: flight spectra

Levin, Penn St: condens., chem. models

SSI: plume reactions

Ketsdever, Wysong, Gimelshein, Young AFRL/PRSA

Boyd, Michigan: particulate models

USC/AFRL facilities: CHAFF, nN stand

Alexeenko, Purdue: new kinetic solvers

Shneider, Princeton: optical lattice theory

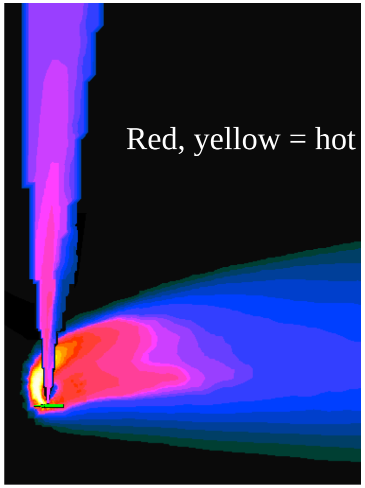
TsNIIMASH Russia: Al2O3 data/models

Ivanov, ITAM Russia: 2-phase, chemistry models

Borisov, USU Russia: gas-surface data

Gov lab
Univ
Int'l
Industry

Innovation in Science: Plume Modeling Recent Accomplishments

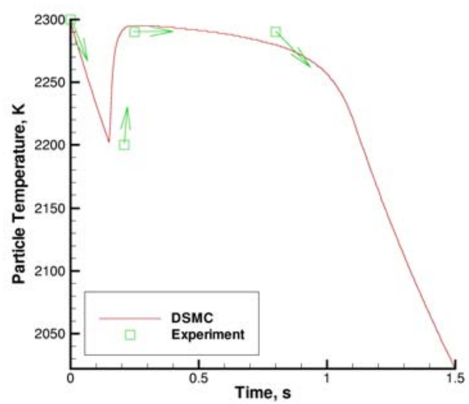


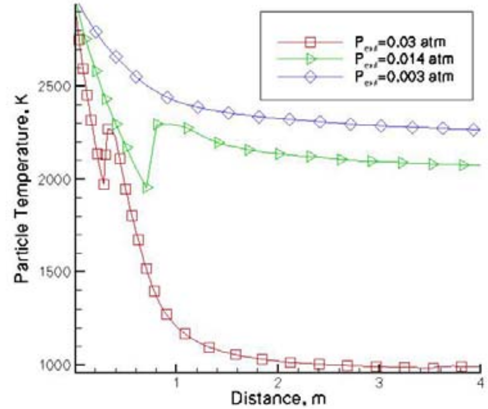
Simulated side-jet 2-phase flow temperature plot: particulates fly in straight line; gas blown back by atmosphere

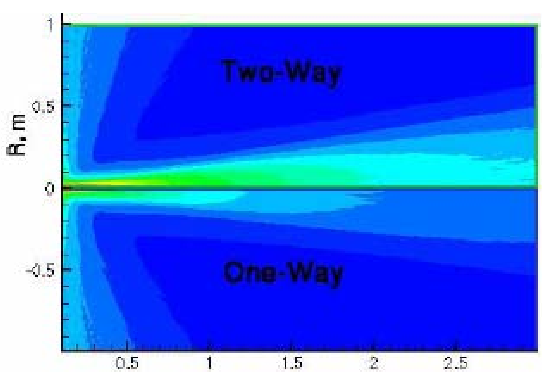
Accomplishments:

Inclusion of particulates / droplets in kinetic (DSMC) simulation is new (2005-2006):

- First coupling of two-phase flow effects into 3D DSMC
- 2 different alumina phase changes included
- Gas-particulate energy accommodation studied –big effect







Plume temperature

Two-way = gas→particle + particle→gas energy coupling

Particulates cool from liquid by radiation (produces α) and kinetic transfer to gas (produces γ)

At appropriate T, liquid-γ change begins from outside at literature-recommended rate

After γ-phase is complete, γ- α transition occurs at recommended rate

Each phase uses recommended emissivity— big effect on signature!!

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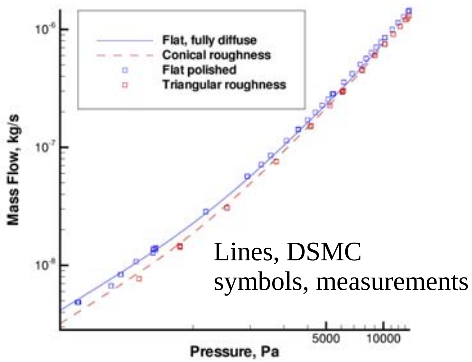
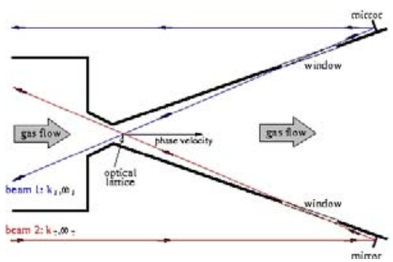
Innovation in Science: MicroFlows

Rough surface effects at a microscale



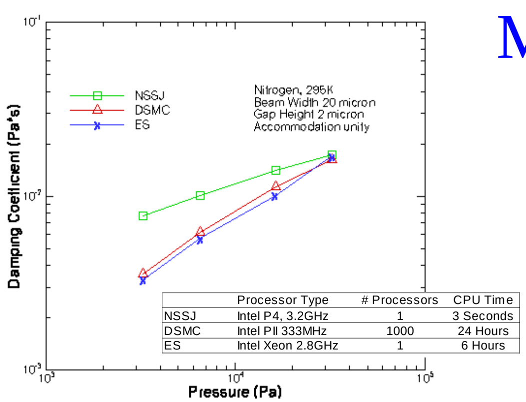
- Efficient surface roughness model developed for particle simulation
- The new model is adapted for use in ES BGK
- Detailed experiments & computations of microchannel flow performed
- New approaches to surface roughness are validated

New microthruster concepts using optical lattices



- High-density microthruster (shown) based on non-resonant energy and momentum deposition from optical lattice to molecular gases
- Low-density microthruster based on acceleration of molecules by optical lattices to tens of kilometers per second

Modeling of damping force on a microbeam



	Processor Type	# Processors	CPU Time
NSSJ	Intel P4, 3.2GHz	1	3 Seconds
DSMC	Intel PII 333MHz	1000	24 Hours
ES	Intel Xeon 2.8GHz	1	6 Hours

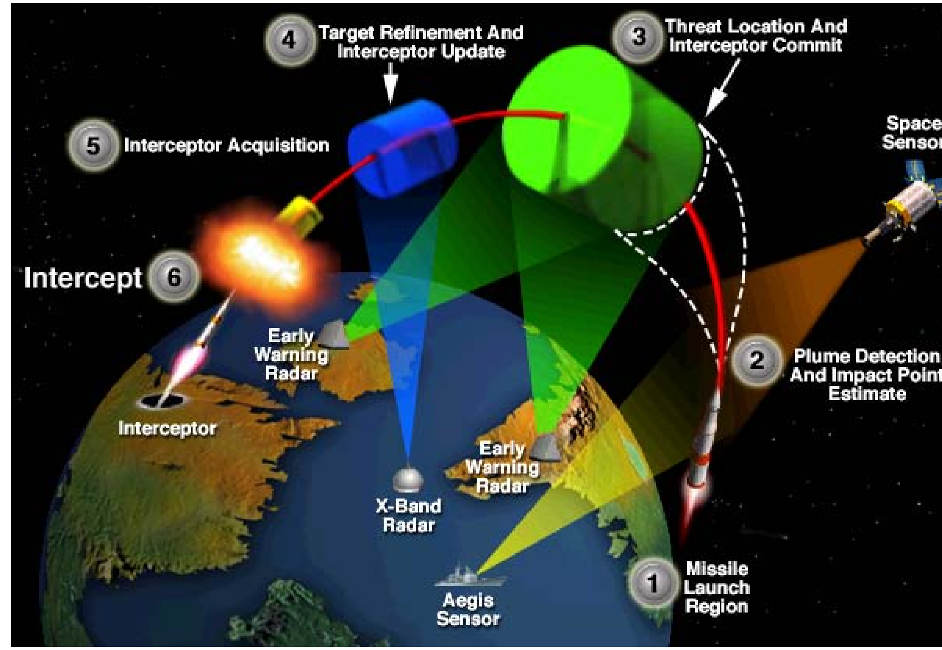
- Accurate solution obtained with ES BGK
- 3 orders of magnitude improvement in computational time compared with DSMC

Damping force per unit length per unit velocity on a microbeam. NSSJ and DSMC: computations by M. Gallis and J. Torczynski of Sandia.

Plume modeling: Impact on Defense and War Fighting Capability

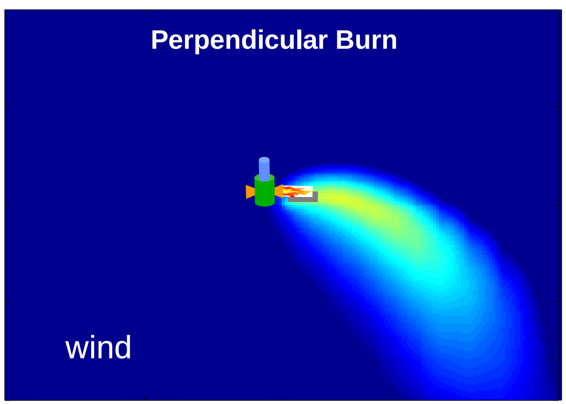
AF need: Accurate "threat missile signature" for all stages of flight is critical for successful missile defense: tracking, kill assessment, sensor design and algorithms

Find, Fix, **Track, Target**, Engage and Assess (F2T2EA)



*courtesy MDA website

Interceptor Sensor Self-Blinding



AFOSR-supported research at AFRL/PRSA has been transitioned – it is currently included in codes being used on projects listed below!

Relevant Air Force and Missile Defense Programs:
Boost Phase Intercept, THAAD, GBI, STSS, Project HERCULES, and SBIRS-HIGH